Propylene glycol diacetate

623-84-7 | DTXSID9044827

Model Performance

Model	
Model	Dala

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)		
Q2	RMSE	R2	RMSE	R2	RMSE	
0.81	0.55	0.81	0.54	0.71	0.61	

Model Results

Predicted value: 1.28

Global applicability domain: Inside

Local applicability domain index: 5.28e-01

Confidence level: 5.99e-01

Nearest Neighbors from the Training Set

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1-Methoxy-2-propyl acetate

Measured: 0.36 Predicted: 8.65e-01

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Urea, 1-(p-fluorophenyl)-

Measured: 1.52 Predicted: 1.70

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N-Methyl-N'-phenylurea

Measured: 1.29 Predicted: 1.47

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Urea, (3-methylphenyl)-

Measured: 1.56 Predicted: 1.57

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Urea, (m-fluorophenyl)-

Measured: 1.77
Predicted: 1.77